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Critical Nucleation Field at the Structured Surface of a Superconductor

by

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CRITICAL NUCLEATION FIELD AT THE STRUCTURED SURFACE OF A SUPERCONDUCTOR

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ABSTRACT

The effect of structured surface of a superconductor on the critical nucleation field is discussed in two cases: one with the magnetic field parallel to the grating wavenumber and the other parallel to the ripples. In the first case, it is found that the critical field is reduced as a function of grating height, whereas in the latter case it is increased.

1. Introduction

The purpose of this paper is to investigate the critical nucleation field (H_{c3}) near the surface of a Ginzburg-Landau (GL) superconductor. We assume that there is a sinusoidal grating imposed on the surface, and the primary purpose of this paper is to investigate the effect that this grating has on the critical field. We shall consider two cases: one in which the external field is parallel to the grating, and the second where the field is perpendicular to the grating.

For a flat surface, this is an old problem, having been previously solved by deGennes.¹ The existence of the grating at the surface complicates the matter by introducing non-trivial boundary conditions, and we shall derive a solution by solving the relevant equation (an elliptic equation) numerically. Thus the primary motivation of this paper is to extend deGennes' work to include roughened surfaces. A secondary motivation is to discover how a rough surface might affect the properties of thin-film superconductors,² especially the new ceramic variety. Unfortunately, the applicability of the GL theory to the new ceramics is questionable. The coherence length appears to be very short, and since the underlying mechanism is not known, it is not at all clear whether the GL theory is the proper phenomenological model. Indeed, recent work by Chela-Flores³ et al constitutes an extension of the GL model which would be appropriate if the resonance valence bond model of superconductivity appears to be accurate. They claim that their new model does reproduce the observed phenomena. Another article by Lobb⁴ demonstrates that the GL theory breaks down close to the critical temperature because of fluctuations.

Therefore, while the direct application of the current work to the new superconductors is problematical, it certainly applies to traditional materials. Further, and this is a subject of ongoing research in this laboratory, the

methods used in this paper are probably readily extendable to the work of Chela-Flores et al. Finally, given that this is an obvious extension of deGennes work, we consider the problem to be of intrinsic interest.

The GL theory is described very nicely by Tinkham,⁵ Schrieffer⁶ and Parks,⁷ in addition to the original paper.⁸ Gor'kov⁹ has shown that the GL theory can be rigorously derived from the BCS theory under the condition that the temperature is close to T_c , the critical temperature. DeGennes has shown that under the appropriate constraints, to be described later, the GL equation reduces to a Schrödinger equation for a harmonic oscillator. The eigenvalues of the equation can be solved analytically, and hence the nucleation field in the bulk (H_{c2}) can be determined. In the reduced units that we are using (which will be described in due course), H_{c2} is found to be $\frac{1}{2\pi}$. DeGennes¹ has shown that, for a flat surface, $H_{c3} = 1/3.71$. We shall duplicate that result in what follows, and also show that a structured surface decreases the surface nucleation field if the magnetic field is oriented parallel to the grating wavenumber. More interestingly, we will also demonstrate that the critical field is increased for the perpendicular orientation.

Section 2 is a description of the GL theory sufficient to define the problem, the notation and the units, while Section 3 contains our result for the case where the external field is parallel to the grating wavenumber. Finally, Section 4 contains the most interesting result, namely the case where the field is perpendicular to the wavenumber.

2. Ginzburg-Landau Theory

In the Ginzburg-Landau theory, a pseudo-wavefunction $\phi(r)$ is introduced as a complex-order parameter. Here $|\phi(r)|^2$ represents the local density of



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superconducting electrons, $n_S(r)$. Near the critical temperature, the free energy of a superconductor can be expanded in powers of $|\phi|^2$ and $|\nabla\phi|^2$. The condition that the free energy must take a minimum value leads to the Ginzburg-Landau equations,

$$\alpha\phi + \beta|\phi|^2\phi + \frac{1}{2m^*}\left(\frac{\hbar}{i}\nabla - \frac{e^*}{c}\vec{A}\right)^2\phi = 0, \quad (2.1)$$

$$\vec{j} = \frac{c}{4\pi} \text{curl } \vec{H} = \frac{e^*\hbar}{2m^*i}(\phi^*\nabla\phi - \phi\nabla\phi^*) - \frac{e^{*2}}{m^*c}\phi^*\phi\vec{A}, \quad (2.2)$$

where m^* and e^* are the mass and charge of the Cooper electron pair, and the parameters ($\alpha < 0$) and β are temperature dependent.

A derivation of the Ginzburg-Landau equation by the variational principle requires certain boundary conditions which have clear physics significance. For an insulating surface, the boundary condition must be¹⁰

$$\left(\frac{\hbar}{i}\nabla - \frac{e^*}{c}\vec{A}\right)\phi|_n = 0, \quad (2.3)$$

where n is the direction normal to the surface. This condition assures that there is no supercurrent in the normal direction of the boundary. For a metal-superconductor interface with no current, deGennes has given the condition¹⁰

$$\left(\frac{\hbar}{i}\nabla - \frac{e^*}{c}\vec{A}\right)\phi|_n = \frac{i}{b}\phi, \quad (2.4)$$

where b is a constant.

If ϕ is much smaller than ϕ_∞ , where $\phi_\infty = (-\alpha/\beta)^{1/2}$ is the value of the wave function in the deep interior of the bulk material, then the β -term in (2.1)

becomes negligible in comparison with the α -term. For this case, one can ignore the β -term and the Ginzburg-Landau equation (2.1) is of the form of a linear elliptic equation. One case to which the linearized Ginzburg-Landau equation can be applied is the nucleation of superconductivity for bulk material with or without a surface. One would like to evaluate the highest field at which superconductivity can nucleate in the interior of a large sample, or near the surface of a bulk sample, in a decreasing external magnetic field. In fact, this is the best case for linearization to be valid. Ideally, at the critical field the superelectron density must be infinitesimal, where the linearized version is accurate. In this instance, the pseudo-wavefunction must decay exponentially into the bulk. The nucleation field in the bulk (H_{c2}) and near a flat surface (H_{c3}) have been found to be¹

$$H_{c2} = \frac{\Phi_0 |\alpha|_m}{\pi \hbar^2} = \frac{1}{2\pi} \left(\frac{\Phi_0}{\xi^2} \right) \quad (2.5)$$

and

$$H_{c3} = 1.695 H_{c2} = 1/1.371 \left(\frac{\Phi_0}{\xi^2} \right) \quad , \quad (2.6)$$

where $\Phi_0 = \frac{hc}{2e}$ is the quantum flux and ξ is the Ginzburg-Landau coherence length.

The Ginzburg-Landau theory is a localized theory of superconductivity, despite the fact that superconducting phenomena are nonlocal. In the Gor'kov derivation of the GL equation from BCS theory, the nonlocality is represented by the symmetric kernel $H_n(\vec{r}, \vec{r}')$, connecting two vectors \vec{r} in coordinate space, where the frequency $\omega_n = (2n+1)T$, and T is the temperature with n ranging over

nonnegative integers. Then, in a dirty superconductor, the mean free path of the bulk material L_0 is much smaller than the Pippard coherence length, and the coherence length for the symmetric kernel in the lowest-frequency approximation is¹⁰

$$\xi_{\omega_0} = \left(\frac{V_F L_0}{6\pi T} \right)^{1/2}, \quad (2.7)$$

where V_F is the Fermi velocity. On the other hand, the Ginzburg-Landau coherence length is proportional to $1/(T-T_c)^{1/2}$, where T_c is the critical temperature. Therefore, as long as $T \rightarrow T_c$, then ξ will be much greater than ξ_{ω_0} and we can neglect the nonlocal effect. In this case, the deGennes boundary condition (2.3) for the free surface would be valid as long as the surface structure is on a scale larger than ξ_{ω_0} . Since the Ginzburg-Landau length can be made arbitrarily long by raising the temperature, we think there is considerable room in which the results derived from using the local approximation will be both valid and interesting, and it is this case that we consider here. In general, the boundary condition is very complicated in as much as the nonlocal effects have to be considered explicitly.^{11,12}

3. Critical Nucleation Field Parallel to Grating Wavenumber

We are interested in knowing the effects of a structured surface on the nucleation critical field H_{c3} . The surface profile function is assumed to be

$$\xi(x) = \gamma \cos(vx), \quad (3.1)$$

where γ is the grating amplitude. For the first case the external field \vec{H} is assumed to be parallel to the grating wavenumber. We assume z to be the distance from the structured surface. By translation symmetry along the y -axis the wavefunction takes the form

$$\phi = e^{ik_y y} f(x, z) \quad (3.2)$$

Then the linearized Ginzburg-Landau equation becomes

$$-\frac{\partial^2 f(x, z)}{\partial x^2} - \frac{\partial^2 f(x, z)}{\partial z^2} + \left(\frac{2\pi H_x}{\Phi_0}\right)^2 (z - z_0)^2 f(x, z) = -\frac{2cm^*}{\hbar^2} f(x, z) \quad (3.3)$$

where we use the gauge $\vec{A} = (0, -H_x z, 0)$ for the vector potential and the boundary condition is

$$\left. \frac{\partial f}{\partial n} \right|_{\text{surface}} = 0 \quad (3.4)$$

In order to obtain the maximum value of H_x , for which $f(x, z)$ has a bound solution, one has to solve the elliptic equation numerically. Then z_0 is an adjustable parameter, and it related to the y -component of the supercurrent expressed as

$$J_y = \left(\frac{e^* \hbar}{m^*} k_y + \frac{e^{*2}}{m^* c} H_x x \right) \phi^* \phi \quad (3.5)$$

we solve the elliptic equation in the over one period of the grating as shown in Fig. 1. The differential equation is replaced by a difference equation.^{13,14}

Assuming periodic boundary conditions, the value of the wavefunction at boundary AO is identical to that of boundary CD. At the surface (boundary AC) we use the von Neumann conditions, i.e., the normal derivative of the wavefunction must be zero. We assume that boundary OD is sufficiently far enough away from the surface so that surface effects can be ignored. We can thus use the analytic solution for the flat surface as the boundary condition here; the value of the wavefunction at this boundary can be an arbitrary constant (normalization condition).

We arrive at the maximum value of H_x for the linearized GL equation by testing the convergence at the bottom boundary (deep in the interior), and also the behavior near the surface. This result corresponds to the bound state of the minimum excitation for a given z_0 . However, z_0 is an adjustable parameter, and one has to vary z_0 in order to maximize the resulting value of H_x . In practice, this results in a two-dimensional variational problem, with the adjustable parameters being H_x and z_0 . We find that, especially for large gratings, the solution can be very unstable to small variations in these parameters, and hence the calculations become quite time consuming. Fig. 2 illustrates a typical result.

Figure 3 shows the numerical result. We have obtained the nucleation critical field H_{c3} for the grating wavenumber about $10\xi^{-1}$ and a grating amplitude ranging from 0 to 1.2 GL coherence lengths. When the grating amplitude is zero, we find $H_{c3} = 1.70H_{c2} = \frac{1.70 \phi}{2\pi\xi^2}$, which is consistent with the result obtained by de Gennes for a flat surface. As the grating height increases, H_{c3} decreases and asymptotically tends toward the value for the bulk material, $H_{c2} = \frac{\phi_0}{2\pi\xi^2}$. This is expected since as the grating height tends to infinity, the structure of the surface becomes a series of superconducting thin films, oriented now parallel to

the z-axis. The direction of the magnetic field is in the x-direction, and hence is oriented vertically with respect to the thin-film layers. The wavefunction must be the bound state with minimum excitation which satisfies (3.5). If $k_x = 0$, then the solution satisfies the von Neumann conditions for the thin film. Thus the critical field must be equated to that for the bulk material, H_{c2} . This ignores the effect in the z-direction, which, however, only affects the region very close to the "top" of the grating. Since the grating amplitude is infinite, this effect can be ignored.

It is also apparent that the critical field does not change significantly for $\lambda < 0.3\xi$. This is because the von Neumann condition forces the wavefunction to be constant near the surface. If the amplitude is much smaller than ξ , then this condition implies that the solution to the GL equation can not vary significantly. As the grating becomes deeper, however, on the order of ξ , then the ripple forces a dramatic change in the value of the wavefunction.

4. Critical Nucleation Field Perpendicular to the Grating Wavenumber

Another interesting case we now consider is the nucleation field in the ripple direction (y-direction). The gauge for the vector potential is

$$\vec{A} = (H_y z, 0, 0) \quad . \quad (4.1)$$

Then the Ginzburg-Landau equation can be written as

$$\begin{aligned} -\frac{\partial^2 f(x,z)}{\partial x^2} - \frac{\partial^2 f(x,z)}{\partial z^2} + \frac{4\pi i H_y z}{\phi_0} \frac{\partial f(x,z)}{\partial x} \\ + \left(\frac{2\pi H_y z}{\phi_0}\right)^2 f(x,z) = \left(-\frac{2m^* \alpha}{\hbar^2} - k_y^2\right) f(x,z) \quad , \end{aligned} \quad (4.2)$$

where we have used the ansatz (3.2) due to translational symmetry along the y -axis. One can rescale the factor $(-\frac{2m^*\alpha}{\hbar^2} - k_y^2)$ of the right-hand side of (4.2) to 1, in which case the quantity $\frac{2\pi H_y}{\phi_0}$ on the left-hand side becomes $\tilde{H}_y = 2\pi H_y / \phi_0 (\frac{2m^*|\alpha|}{\hbar^2} - k_y^2)$. If one finds the maximum value \tilde{H}_{yc} at which a bound solution of (4.2) exists, then the corresponding critical nucleation field is

$$H_{c3} = \tilde{H}_{yc} \frac{\phi_0 |\alpha| m^*}{\pi \hbar^2}, \quad (4.3)$$

with

$$k_y = 0, \quad (4.4)$$

which is similar to the previous cases.

We numerically solve the elliptic equation (4.2) by the same technique described in Sec. 3. The only difference is the boundary condition at the structured surface, written as

$$\frac{\partial f}{\partial n} = \frac{ie^*}{\hbar c} A_n f. \quad (4.5)$$

Figure 4 shows the numerical result. We have obtained the nucleation critical field H_{c3} for the grating wavenumber about $10\xi^{-1}$ and a grating amplitude ranging from zero to 0.6 GL coherence lengths. Of course, when the grating amplitude is zero, we recover the deGennes result for a flat surface. Unlike the case for which the external field is parallel to the grating wavenumber, here the calculation shows that the critical field increases as a function of grating

amplitude. It is expected that the value of the critical field will reach the value for superconducting films, with a thickness of the same order as the period of the structure. It is noted that if the thickness of a film is much smaller than the London coherence length, the critical field must be much greater than the bulk value.

ACKNOWLEDGMENTS

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Figure Captions

- Fig. 1 A schematic drawing of the system under discussion. Letter O refers to the origin of our coordinate system. The nature of the boundaries is described in the text. The amplitude of the grating is γ , whereas the wavelength is 0.6ξ .
- Fig. 2 This shows the wavefunction at the nucleation critical field for a structured surface. Here $\gamma = 0.22\xi$, $\nu = \frac{2\pi}{0.6\xi}$ and $H_{c3} = \frac{0.26\phi_0}{\xi^2}$ and $z_0 = 0.64\xi$. While the amplitude of the wavefunction is determined by an arbitrary normalization constant, close inspection shows that the magnitude of the electron density decreases in the ripples.
- Fig. 3 Nucleation critical field vs. grating amplitude for a field oriented parallel to the grating wavenumber. The amplitude is measured in units of the GL coherence length whereas the critical field is in units $\frac{\phi_0}{\xi^2}$. The wavenumber of the grating is about $10/\xi$ (see text).
- Fig. 4 Nucleation critical field vs. grating amplitude for a field oriented parallel to the ripples. Units are the same as in Fig. 3.

Fig. 1

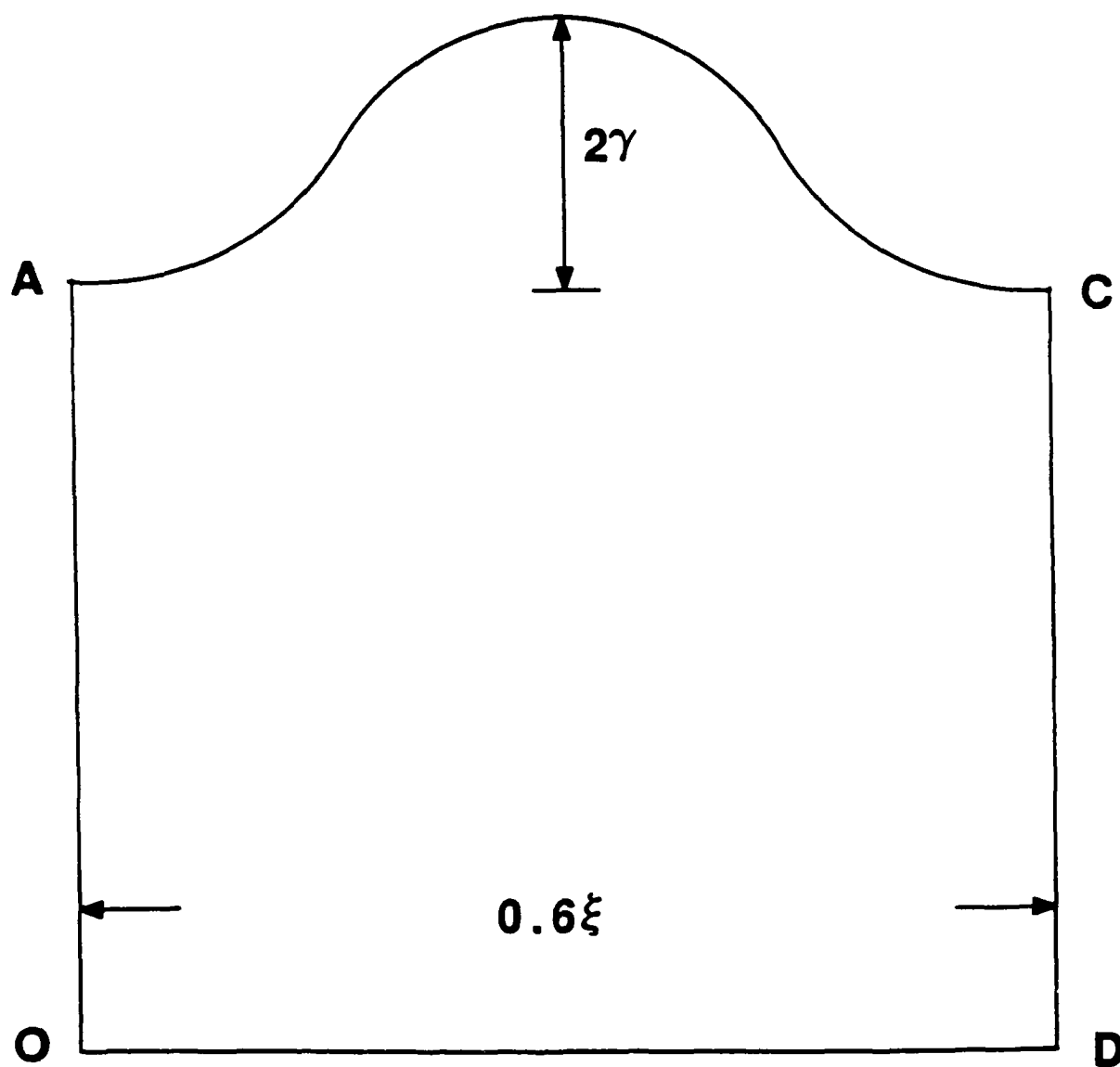


Fig. 2

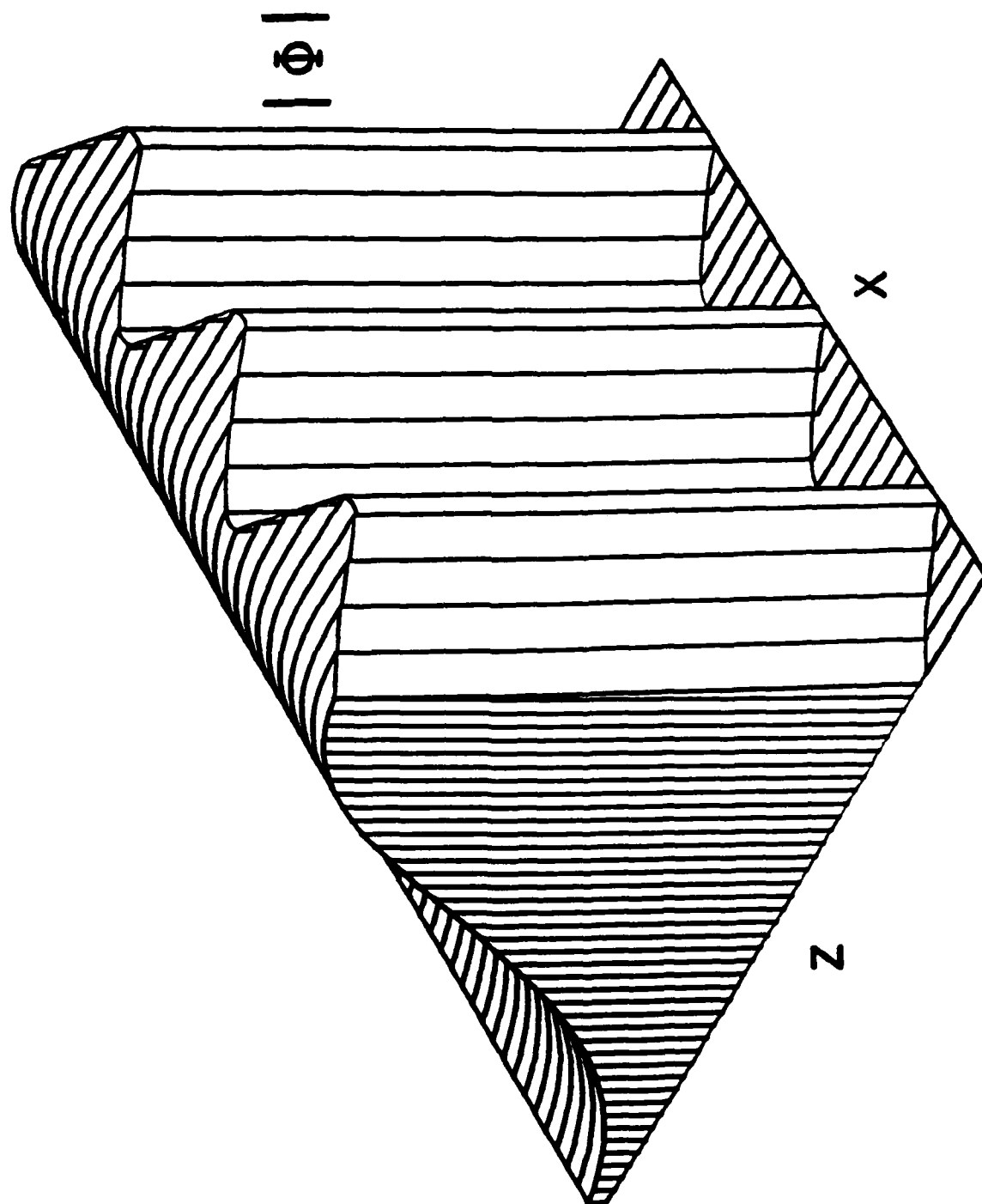


Fig. 3

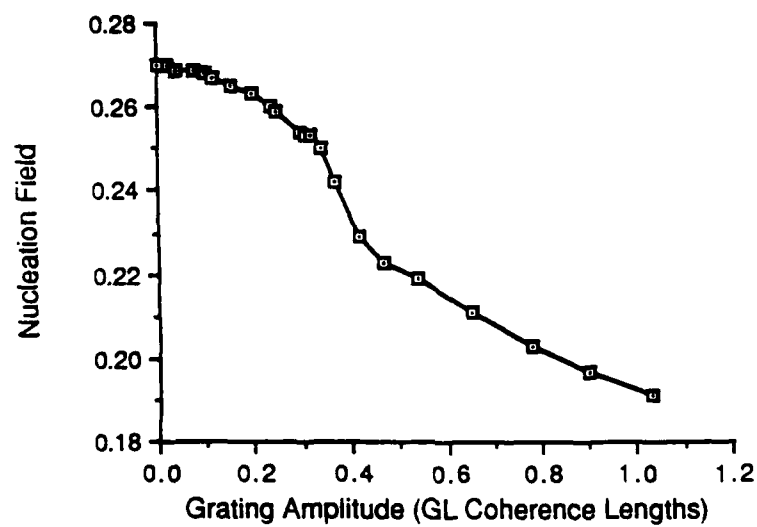
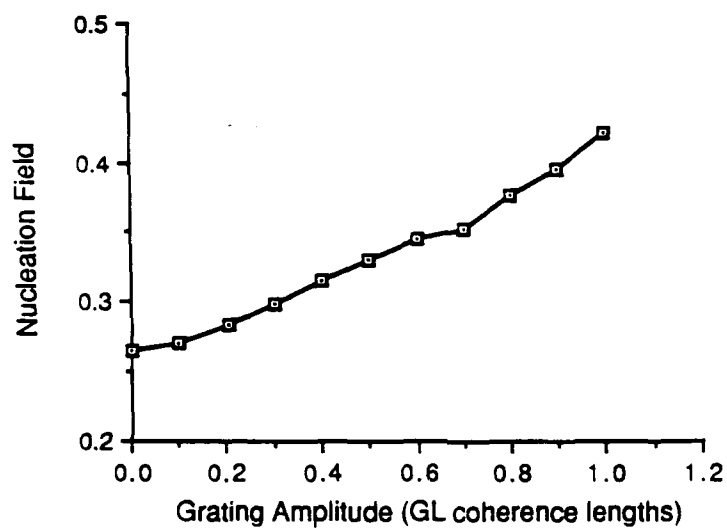


Fig. 4



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